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Maximum Limit of Rotational Energy Transfer on O_2 Collision with He and Hard Ellipsoid Potential Model

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ABSTRACT

The importance of power-gap law which is treat as well known parameter $|\Delta E|^*$ given by two parameters and the classical limit of the maximum rotational energy transfer, $(\Delta E)_{max}$, has been reviewed for a two dimensional hard ellipsoid potential model over a wide range of energies of the system. It has been found that $(\Delta E)_{max}$, predicted by the hard ellipsoid potential is comparable to a well-known parameter $|\Delta E|^*$. The numerical equivalence of $(\Delta E)_{max}$ and $|\Delta E|^*$ has been verified for different collision energy of the system. Such equivalence suggests that the value of $(\Delta E)_{max}$ can be used as one parameter $|\Delta E|^*$ of the power -gap law.

Keywords: Rotational energy transfer, Diatomic collision and scattering cross section.

1. INTRODUCTION

The study of rotational inelastic scattering between molecules and neutral atoms at low collision energies is a fast developing field in collision dynamics[1-3]. The nature of rotational energy transfer (RET) in collisions of molecules with He, Ar and Ne were studied experimentally[4-6] and theoretically[7-9].

In several papers Mc caffery and co-workers[10-12] explored various aspects of the RET by treating the conversion of orbital angular momentum to the angular momentum of the molecule at the repulsive wall of anisotropic intermolecular potential.

However they point out that the maximum change in rotational momentum might be limit either by energy conservation or by momentum conservation, developing on detail of the particular collision system. They obtain the maximum classical limit of RET by using a hard ellipsoid potential model. This model treats a molecule as a hard core ellipsoid and the collision between the atom and the hard core ellipsoid.

The relationship between the shape of the potential surface and the energy transfer is crucial for understanding collision processes of molecules and atoms. The link between the two is provided by the general quantum theory of collision for hard shapes. The problem of the rotationally inelastic collision of a particle with a hard ellipsoid potential[13-14] can be solved by using the three principles of conservation; the total energy conservation, linear momentum conservation and the angular momentum conservation. Agrawal and co-workers[15-18] have noted that the classical limit of rotational energy transfer $(\Delta E)_{max,}$ predicted by the hard ellipsoid model is comparable to a well known parameter $|\Delta E|^*$ given by power - gap law[19] and the RET cross –sections computed on the real potentials.

It would be important to perform an elaborate test of the expression for the maximum limit of angular momentum transfer so obtained, such a test would be useful for the RET cross- sections computed using the realistic potential.

In this study, in addition to the validity of the hard ellipsoid potential model we shall also reconfirm that the division between the classically allowed and forbidden transitions given by the power-gap law is excellent. Further, we show that the equivalence of the $|\Delta E|^*$ and $(\Delta E)_{max,}$ not only provide the physical meaning to $|\Delta E|^*$ given by the RET data and the power -gap law but is also valuable for determination of some features of intermolecular interaction potential from knowledge of RET data.

In Section 2, we formulate the procedure for determination of $|\Delta E|^*$ and $(\Delta E)_{max}$. The numerically results are presented and discussed in Section 3. Finally the conclusions are summarized in Section 4.

2. FOMULATION

2.1. Determination of lΔEl*

The parameter $|\Delta E|^*$ is determined with the help of cross sections obtained from scattering calculations and the power gap law.

For the computation of cross sections the homonuclear diatomic molecule, O2, is treated as a rigid rotor and the interaction between the molecule and the atom, He, is taken as a pairwise sum of the potential terms,

$$V = V(r_1) + V(r_2) \quad (1)$$

where r_1 and r_2 are the O^1-He and O^2-He distances, respectively, as shown in Fig.1.

For $V(r_i)$ the general form of the Lennard–Jones (L-J) potential is taken with different values of n and m:

$$V(r_i) = \varepsilon[\{m/(n-m)\}(r_o / r_i)^n - \{n/(n-m)\}(r_o / r_i)^m], \ (i = 1, 2), \quad (2)$$

where r_0 and ε are taken[19] as 1.2074 Å and 2.98928 meV, respectively .

In addition to the above-mentioned potential functions, purely repulsive terms of the potential functions have also been investigated. It is convenient to denote such potentials by the notation $V_R(n)$, which has been obtained by deleting the attractive term from the potential V (n, m). The cross sections have been computed using the modified infinite order sudden approximation method (IOSAM),[20]. The phase shifts have been computed using a 10-point Gauss – Mehler quadrature of the WKB phase shift equation as described by Pack[21].

According to the power gap law[19] the cross sections, $\sigma (j_i \rightarrow j_f)$ can be expressed as

$$\sigma (j_i \rightarrow j_f) = a (2 j_f + 1) (T_f/T_i)^{1/2} \left| \Delta E \right|^{-\gamma} \quad (3)$$

where j_i and j_f are the initial and final rotational quantum numbers, a and γ are the fitting parameters, T_f and T_i are the final and initial translational energies and lΔEl is the energy gap between initial and final rotational levels. Eq. (3) gives the following equation which can be used to separate the two regions.

$$Y = - \gamma X + \text{In } a \quad (4)$$

where

$$Y = \ln [\sigma (j_i \rightarrow j_f) (T_i/T_f)^{1/2} / (2 j_f + 1) \quad (5)$$

and

$$X = \ln |\Delta E|^{*}. \quad (6)$$

A typical X-Y plot which shows the existence of two straight lines signifying the two regions is given in Fig. (2). The location of the critical point has been marked as $|\Delta E|^{*}$ in the figure. For all sets of the computed cross sections, $|\Delta E|^{*}$ has been obtained by such plots.

2.2. Determination of $(\Delta E)_{max}$

For the maximum limit of angular momentum transfer the hard ellipsoid potential model was discussed in detailed by Agrawal and co-workers[15-18]. He found the following relation for the classical limit of the angular momentum transfer

$$(\Delta J)_{max} = \sqrt{(2\mu)}(\sqrt{E}+\sqrt{E'}) (A-B) \quad (7)$$

where μ is the reduced mass of the colliding system, E and E' are the initial and final translational energies of the system, respectively and A and B are the lengths of the semi – major and semi-minor axes of ellipsoid, respectively.

From the above expression the limit of the rotational energy transfer in the molecule can easily be obtained. For simplicity, if the diatomic molecule is considered initially in the ground state, then the expression for the maximum amount of rotational energy transfer would be

$$(\Delta E)_{max} = [(\Delta J)_{max}]^{2} / 2I,$$
$$(\Delta E)_{max} = (\mu / I) (A-B)^2 [E+E' + 2\sqrt{(EE')}] \quad (8)$$

where I is the moment of inertia of the diatomic molecule. Eq. (8) together with the following energy conservation equation

$$E' = E - (\Delta E)_{max}, \quad (9)$$

can be used to compute $(\Delta E)_{max}$ from knowledge of E, A, B, μ and I.

3. RESULTS AND DISCUSSION EFFECT OF ENERGY

Table 1 list γ_{low}, γ_{high} and $|\Delta E|^*$ given by the scattering calculations for the potential V (12, 6) and V_R (6) as a function of the initial translational energy for O_2- He system. For comparison the value of $(\Delta E)_{max}$ given by Eq. (8) are also shown in the Table 1. A comparison of the values of $(\Delta E)_{max}$ given by the hard ellipsoid model and $|\Delta E|^*$ given by the scattering method shows that they are in very good agreement. This excellent agreement shows that $|\Delta E|^*$ can be considered as $(\Delta E)_{max}$.

The data reported in Table 2 also shows that $(\Delta E)_{max}$ is approximately proportional to E : $(\Delta E)_{max}$ / E varies from 0.033 to 0.182 as E increases from 0.1 to 0.5 eV. The variation of $(\Delta E)_{max}$ / E with E can be analyzed by the two factors $(A-B)^2$ and $[E+E' + 2\sqrt{(EE')}]$ / E, occurring in Eq. (8). The factor $(A-B)^2$ decreases from 0.3199 to 0.3785 and letter factor increases from 2.3664 to 1.8898 as E increases from 0.1 to 0.5eV. For a perfectly hard ellipsoid potential, $(A-B)^2$ would not depend on E and as such the variation in $(\Delta E)_{max}$ / E would be given by the later factor only. Another important parameter is, γ. For a given potential we see that γ_{low} is insensitive to the change in the collision energy. The values of γ_{high}, however, shows a different trend. The energy dependence of these parameters is a matter of further studies.

Table-T_1

Comparing of maximum amount of rotational energy transfer $(\Delta E)_{max}$ values by the hard ellipsoid potential model and those obtained by using the scattering cross sections and the power- gap law for the O_2-He system.

Potential	Energy (eV)	γ_{low} [(a)]	γ_{high} [(a)]	$(\Delta E)_{max}$ eV.	
				Ellipsoid Model	Scattering
V (12 ,6)	0.10	0.788	7.56	0.032	0.033
	0.15	0.846	9.29	0.048	0.054
	0.20	0.813	9.38	0.065	0.068
	0.25	0.803	9.24	0.077	0.082
	0.30	0.803	8.98	0.098	0.095
	0.35	0.807	9.86	0.122	0.115
	0.40	0.814	10.61	0.140	0.135
	0.45	0.822	10.91	0.161	0.152
	0.50	0.793	9.96	0.190	0.182
V_R(12)	0.10	1.0	8.89	0.027	0.032
	0.15	0.887	8.66	0.042	0.044
	0.20	0.855	8.65	0.056	0.056
	0.25	0.844	8.57	0.070	0.069
	0.30	0.842	8.19	0.086	0.081
	0.35	0.844	9.12	0.101	0.100
	0.40	0.848	9.94	0.116	0.119
	0.45	0.854	10.56	0.132	0.137
	0.50	0.828	9.91	0.148	0.148

(a) The unit of γ_{low} and γ_{high} are such that in Eq. (3) cross section is in $(Å)^2$ and ΔE is in eV.

Table-T_2

Comparing of maximum amount of rotational energy transfer $(\Delta E)_{max}$ values by the hard ellipsoid potential model and those obtained by using the scattering cross sections for the O_2-He system.

Potential	Energy (eV.)	A Å	B Å	A-B Å	$(\Delta E)_{max}$ eV.	
					Ellipsoid Model	Scattering
V (12 ,6)	0.10	2.9320	2.3664	0.5656	0.032	0.033
	0.15	2.8670	2.3006	0.5664	0.048	0.054
	0.20	2.8214	2.2528	0.5686	0.065	0.068
	0.25	2.7656	2.2156	0.5500	0.077	0.082
	0.30	2.7564	2.1848	0.5716	0.098	0.095
	0.35	2.5190	1.9250	0.5940	0.122	0.115
	0.40	2.4998	1.9046	0.5982	0.140	0.135
	0.45	2.5006	1.8984	0.6022	0.161	0.152
	0.50	2.5050	1.8898	0.6152	0.190	0.182
$V_R(12)$	0.10	3.0052	2.4700	0.5352	0.027	0.032
	0.15	2.9254	2.3830	0.5424	0.042	0.044
	0.20	2.8702	2.3230	0.5472	0.056	0.056
	0.25	2.8284	2.2774	0.5510	0.070	0.069
	0.30	2.7948	2.2406	0.5542	0.086	0.081
	0.35	2.7670	2.2100	0.5570	0.101	0.100
	0.40	2.7430	2.1836	0.5594	0.116	0.119
	0.45	2.7220	2.1606	0.5614	0.132	0.137
	0.50	2.7134	2.1484	0.5650	0.148	0.148

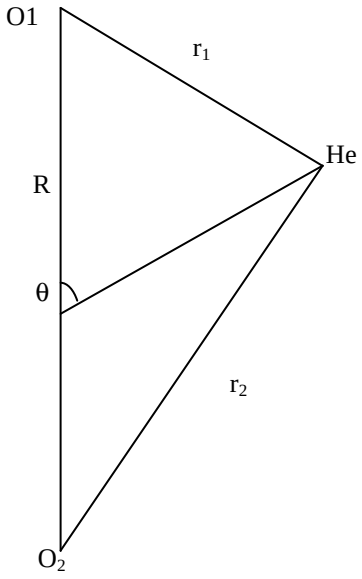

Fig.(1) Coordinates for the rigid rotor F_2-He system

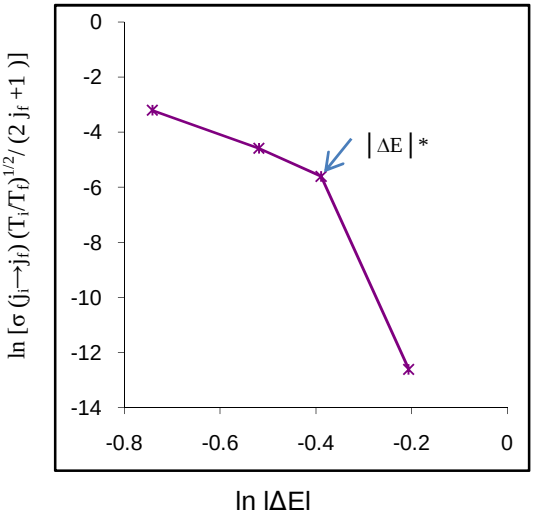

Fig. (2) ln [σ ($j_i \rightarrow j_f$) $(T_i/T_f)^{1/2}$/ (2 j_f +1) versus ln lΔEl for j_i=0 at E= 0.1 eV for V_r(12) potential. lΔEl* point is shown by an arrow. The unit of ΔE and σ are eV and Å, respectively.

CONCLUSION

The maximum amount of rotational energy transfer in collisions of O_2 with He has been investigated over a wide range of energies, reduced mass of the system, potential functions and potential parameters. Further, the classical limit of maximum rotational energy transfer has been reviewed for a hard ellipsoid potential model.

The $|\Delta E|^{*}$ * values obtained by scattering results are compared with those given by $(\Delta E)_{max.}$ values predicted by the hard ellipsoid potential model. The good agreement between $|\Delta E|^{*}$ and $(\Delta E)_{max}$ values over the wide range of energies and different potential functions suggest that the parameter $|\Delta E|^{*}$ given by power-gap law has a physical significance, $|\Delta E|$* is nothing but the classical limit of the rotational energy transfer. Further, the equivalence of $|\Delta E|^{*}$ and $(\Delta E)_{max}$ also suggest that the classical limit of angular momentum transfer given by the hard ellipsoid potential model is meaningful even for the cross sections computed on the real potentials provided the classical turning point surface of the soft potential is assumed as the hard potential surface. The $l\Delta El^{*}$ values given by the scattering results are also found to be in good agreement with the $(\Delta E)_{max}$ values obtained by using the hard ellipsoid model.

Similarly, the dependence of $(\Delta E)_{max}$ for O_2-He system has been investigated for different types of potential surfaces over a wide range of initial collision energy and potential parameters. In all cases it is found that the agreement between $(\Delta E)_{max}$ and $|\Delta E|^{*}$ is good to excellent. The agreement, however, is not so good for the potentials having large well depth.

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